Elementary excitations of the symmetric spin-orbital model: The XY limit

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The elementary excitations of the 1D, symmetric, spin-orbital model are investigated by studying two anisotropic versions of the model, the pure XY and the dimerized XXZ case, with analytical and numerical methods. While they preserve the symmetry between spin and orbital degrees of freedom, these models allow for a simple and transparent picture of the low–lying excitations: In the pure XY case, a phase separation takes place between two phases with free–fermion like, gapless excitations, while in the dimerized case, the low-energy effective Hamiltonian reduces to the 1D Ising model with gapped excitations. In both cases, all the elementary excitations involve simultaneous flips of the spin and orbital degrees of freedom, a clear indication of the breakdown of the traditional mean-field theory.

The impact of orbital degeneracy on the low–energy properties of Mott–Hubbard insulators is currently attracting a lot of attention following the progress in synthetizing and studying materials with these characteristics [1]. It was already pointed out a long time ago by Kugel and Khomskii that such systems should have low–lying orbital excitations in addition to spin excitations [2]. More recently, it has been suggested that the interplay between both degrees of freedom can have more dramatic consequences. For instance, under suitable conditions the orbital degeneracy can enhance quantum fluctuations in the spin degrees of freedom and lead to gapped spin excitations even in the 3D case [3]. Another interesting situation is the SU(4) symmetric case [4,5] where the system cannot choose locally between the configurations (spin singlet × orbital triplet) and (spin triplet × orbital singlet). Then the mean-field approach that decouples spin and orbital degrees of freedom on each bond cannot be a good starting point in that case since it violates basic SU(4) relationships between correlation functions on a given bond, as emphasized in Ref. [6]. As a consequence, the traditional picture of relatively independent spin and orbital excitations must be abandoned. A clear picture of the low-lying excitations in such a case is still lacking though.

In this Letter, we concentrate on the symmetric case. The basic model is the SU(4) symmetric Hamiltonian given by

$$H = J \sum_i \left(2\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{2}\right)\left(2\vec{\tau}_i \cdot \vec{\tau}_{i+1} + \frac{1}{2}\right) \qquad (1)$$

where $\vec{S}_i$ and $\vec{\tau}_i$ are spin-1/2 operators corresponding to spin and orbital degrees of freedom respectively. This model has already been studied rather extensively by several methods [4–9]. In particular, it is known from the Bethe ansatz solution that there are three branches of low-energy excitations [7]. The physical interpretation of these branches is not straightforward though. The essential complexity comes from the large local degeneracy: For a single bond, the groundstate is six-fold degenerate (spin singlet × any of the three orbital triplets or any of the spin triplets × orbital singlet). It is thus interesting to study the XXZ version of the model defined by

$$H = \sum_i J_i \left(2(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z) + \frac{\lambda}{2}\right) \times \left(2(\tau_i^x \tau_{i+1}^x + \tau_i^y \tau_{i+1}^y + \lambda \tau_i^z \tau_{i+1}^z) + \frac{\lambda}{2}\right) \qquad (2)$$

In that case, the degeneracy is lifted within the triplet sector as soon as $\lambda < 1$, and the groundstate of a given bond is only two-fold degenerate (spin singlet × orbital triplet with $\tau^z_{tot} = 0$ or spin triplet with $S^z_{tot} = 0$ × orbital singlet). The essential ingredient, namely the symmetry between spin and orbital degrees of freedom, is preserved, but the Hilbert space of the low-lying sector is considerably reduced.

In the following, we will concentrate on two versions of this model for which a transparent picture of the low-lying excitations can be obtained:

The pure XY model: It corresponds to the previous Hamiltonian [Eq. (2)] with $\lambda = 0$ and $J_i = J$ for all bonds, which can be written more compactly as

$$H = J \sum_i \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)\left(\tau_i^+ \tau_{i+1}^- + \tau_i^- \tau_{i+1}^+\right) \qquad (3)$$

or in expanded form

$$H = J \sum_i \left(S_i^+ \tau_i^+ S_{i+1}^- \tau_{i+1}^- + S_i^- \tau_i^- S_{i+1}^+ \tau_{i+1}^+\right) + J \sum_i \left(S_i^+ \tau_i^- S_{i+1}^- \tau_{i+1}^+ + S_i^- \tau_i^+ S_{i+1}^+ \tau_{i+1}^-\right). \qquad (4)$$

Analyzing this hamiltonian in the product basis $\otimes_i |\eta\rangle_i$, where $|\eta\rangle_i = |S_i^z = \pm\frac{1}{2}, \tau_i^z = \pm\frac{1}{2}\rangle$ and denoting

$$|a\pm\rangle_i = |S_i^z = \pm 1/2,\, \tau_i^z = \pm 1/2\rangle,$$
$$|b\pm\rangle_i = |S_i^z = \pm 1/2,\, \tau_i^z = \mp 1/2\rangle, \qquad (5)$$

one can easily show that all the matrix elements of H between states $\{|a\pm\rangle_i\}$ and $\{|b\pm\rangle_j\}$ vanish. As a consequence, the eigenstates can be classified according to the sequence of domains of *phase A* (with parallel orbital and spin states) and *phase B* (with antiparallel states) that include only states of type $|a\pm\rangle_i$ and $|b\pm\rangle_i$ respectively, and Eq. (4) can be written as

$$H = 2J \sum_i \frac{1}{2}(\alpha_i^+ \alpha_{i+1}^- + \alpha_i^- \alpha_{i+1}^+)$$
$$+2J \sum_i \frac{1}{2}(\beta_i^+ \beta_{i+1}^- + \beta_i^- \beta_{i+1}^+), \qquad (6)$$

where $\alpha_i^\pm = S_i^\pm \tau_i^\pm$ ($\beta_i^\pm = S_i^\pm \tau_i^\mp$) are the raising and lowering spin-1/2 operators corresponding to $|a\pm\rangle_i$ ($|b\pm\rangle_i$). Now the Hamiltonian within a phase can be mapped onto spinless fermions with a Jordan–Wigner transformation, and the groundstate energy of a domain of length L is given by

$$E(L) = -2J \cos\left(\frac{(L/2+1)\pi}{2(L+1)}\right) \frac{\sin\left(\frac{(L/2)\pi}{2(L+1)}\right)}{\sin\left(\frac{\pi}{2(L+1)}\right)} \qquad (7)$$

It is easy to check that $E(L) < E(L_1) + ... + E(L_n)$, where $L_1, ..., L_n$ are integers such that $L_1 + ... + L_n = L$. So the model of Eq. (6) undergoes a phase separation, and the groundstate is two-fold degenerate with a single domain of phase A or B.

The phase separation has some drastic consequences for the thermodynamics, and the low-temperature properties of the pure XY spin-orbital model turn out to be significantly different from those of the SU(4) symmetric model [Eq. (1)]. In Fig. 1 we show the entropies s per site as a function of temperature for both models, the SU(4) symmetric model [Eq. (1)] and the pure XY-case [Eq. (3)]. They have been calculated numerically for chains of length $L = 200$ with periodic boundary conditions, using the continuous time quantum Monte Carlo loop algorithm [10,11]. At very low temperature, both entropies show a linear behavior (see inset of Fig. 1), indicating the presence of gapless excitations. But the slope for the SU(4) is much larger than that in the pure XY spin-orbital case. In fact, in the first case the slope is three times bigger than that of single SU(2) antiferromagnetic Heisenberg chain [6], while the slope of the entropy at low T in the pure XY spin-orbital model is equal to that of the XY model with coupling $2J$, as expected from Eq. (6). A further difference is visible as the temperature is increased. The entropy of the SU(4) symmetric spin-orbital model remains approximately linear also in the intermediate temperature range (up to $T \approx 0.2J$). The entropy of the pure XY spin-orbital model, on the other hand, coincides with the linear behavior of the XY-model only up to a crossover temperature $T^* \approx 0.05J$. Above T^* a sharp increase of the entropy takes place (see inset of Fig. 1). This increase comes from the additional entropy contribution of the domain walls which are more and more frequent with increasing temperature. This can be seen in Fig. 2 where the average density of domain walls p (average number of domain walls per site) is depicted as a function of temperature. Up to T^*, the spin-orbital model is in one of the phases A or B and $p = 0$ within the statistical errors of the Monte Carlo simulation. Above T^* the number of phase sectors increases very sharply with increasing T.

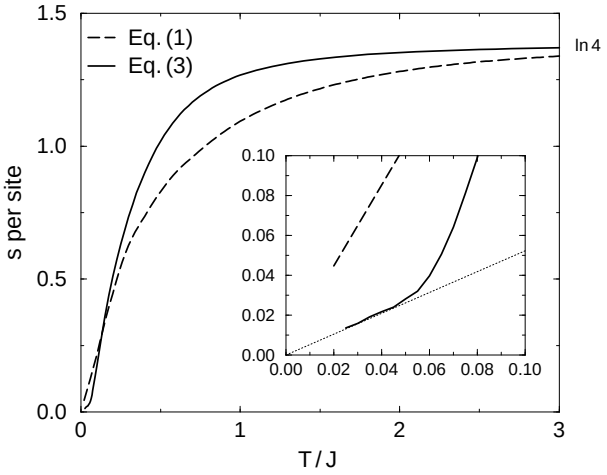

FIG. 1. Temperature dependence of the entropy of the SU(4) symmetric spin orbital model of Eq. (1) (dashed line, taken from Ref. [6]) and of the pure XY spin-orbital model of Eq. (3) (solid line) for chains of length $L = 200$ with periodic boundary conditions in two different temperature scales. For comparison the analytical result for the entropy of the XY-model with coupling $2J$ and infinite length is also shown (dotted line).

This behaviour can be easily understood in terms of the following, approximate free energy per site:

$$f(T,p) = pE_{DW} - Ts_{DW}(T,p) - Ts_D(T) \qquad (8)$$

The various quantities entering this expression are: i) p, the concentration of domain walls, to be determined by minimizing the free energy; ii) E_{DW}, the energy of a domain wall. This is the energy required to split a finite chain of length L into two chains of length $L - L_1$ and L_1, i.e. $E(L - L_1) + E(L_1) - E(L)$, where $E(L)$ is defined in Eq. (7). E_{DW} is *a priori* a function of L and L_1. It turns out that, for large enough L, $E_{DW} \simeq 0.36J$ regardless of L and L_1 except for $L_1 < L_0 \simeq 20$. Since L_0 does not depend on L, this difference will play no role in the thermodynamic limit at low temperatures, and one can safely assume $E_{DW} = 0.36J$; iii) $s_{DW}(T,p)$, the

entropy of the domain walls. For small p, it is given by $s_{DW}(T,p) = -p \ln p$; iv) $s_D(T)$, the entropy contribution of the domains. When p is small, finite-size effects are negligible, and $s_D(T)$ is equal to the entropy of the XY model with coupling $2J$, i.e. $(\pi/6)(T/J)$ at low temperature.

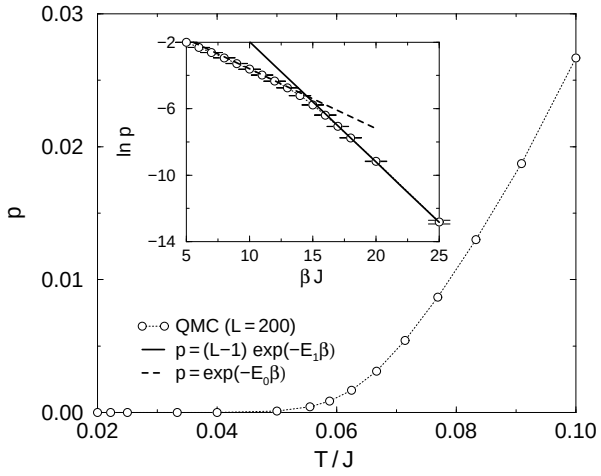

FIG. 2. Temperature dependence of the average density p of domain walls in the pure XY spin-orbital model. The error bars are smaller than the symbols. The inset shows $\ln p$ as function of the inverse temperature βJ as well as fits of the form $p = \exp(-E_0/T)$ and $p = (L-1)\exp(-E_1/T)$ in the intermediate and very low temperature ranges (for details see text).

As for the 1D–Ising model, minimizing with respect to the density of domain walls p leads to $p = \exp(-E_{DW}/T)$ and $s_{DW}(T) = (E_{DW}/T)\exp(-E_{DW}/T)$. The total entropy, which is the sum of $s_{DW}(T)$ and $s_D(T)$, is then dominated at low temperature by $s_D(T) \simeq (\pi/6)(T/J)$, while the domain wall contribution takes over at higher temperature. To be more quantitative, let us define the temperature T_1 where both contributions are equal. It is given by $(E_{DW}/T_1)\exp(-E_{DW}/T_1) = (\pi/6)(T_1/J)$, which leads to $T_1 = 0.074J$. This is in very good agreement with the numerical results of Fig. 1.

The prediction for the density of domain walls is also in very good agreement with the numerical simulations (see inset of Fig. 2, dashed line) for not too low low temperatures: A fit with an exponential law $p = \exp(-E_0/T)$ for $8 \leq \beta \leq 12$ gives $E_0 = 0.36(1)$, in very good agreement with the domain-wall energy E_{DW}. For very low temperatures, namely for temperatures where the average number of domain walls is of order 1 or smaller, and for finite systems, the above picture cannot work because the numerical simulations were performed using periodic boundary conditions, and domain walls can be created only by pairs with a minimum energy $2E_{DW}$. Neglecting configurations with more than one pair of domain walls, one can show that the concentration is expected to behave like $p \simeq (L-1)\exp(-2E_{DW}/T)$. A fit of the very low temperature numerical data could indeed be performed with the law $p = (L-1)\exp(-E_1/T)$ for $15 \leq \beta \leq 25$ (see inset of Fig. 2) with $E_1 = 0.72(2)$, again in very good agreement with $2E_{DW}$. Note that the temperature T_0 below which finite-size effects due to periodic boundary conditions start to influence the thermodynamics is given by $\exp(-E_{DW}/T_0) = 1/L$, i.e. $T_0 \simeq E_{DW}/\ln L$. Since it vanishes when the system size goes to infinity, the free energy of Eq. (8) is expected to be valid down to zero temperature in the thermodynamic limit.

To summarize this section, the very low temperature excitations correspond to simultaneous flips of spin and orbital degrees of freedom within one domain, and domain wall excitations corresponding to collective excitations involving spins and orbital degrees of freedom play an important role above a cross-over temperature $T^* \simeq 0.05J$.

The dimerized XXZ model: It corresponds to the Hamiltonian of Eq. (2) with $J_i = J$ if i is even and $J_i = \alpha J$ if i is odd. We wish to study that model in the limit $\alpha \ll 1$. Let us start by introducing some notations. The Hilbert space of a given bond is spanned by the 16 states $|SS\rangle$, $|ST_i\rangle$ $(i=-1,0,1)$, $|T_iS\rangle$ $(i=-1,0,1)$ and $|T_iT_j\rangle$ $(i,j=-1,0,1)$, where the first (second) letter refers to the spins (orbitals), while $|S\rangle$ and $|T_i\rangle$ are the usual singlet and triplets given by $|S\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, $|T_1\rangle = |\uparrow\uparrow\rangle$, $|T_0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ and $|T_{-1}\rangle = |\downarrow\downarrow\rangle$. In the pure Heisenberg case, the six states $|ST_i\rangle$ and $|T_iS\rangle$ $(i=-1,0,1)$ are degenerate groundstates. However this degeneracy is partially lifted if $\lambda < 1$ in Eq.(2), and the groundstate of a given bond is only two–fold degenerate ($|ST_0\rangle$ and $|T_0S\rangle$). If $\alpha = 0$, the groundstate of Eq.(2) is then $2^{L/2}$–fold degenerate, where L is the number of sites, since each dimer $(i,i+1)$, i even, can be in any of the two states $|ST_0\rangle_i$ or $|T_0S\rangle_i$. Let us study how this degeneracy is lifted when α is switched on. Since we have a two-level system on each dimer $(i,i+1)$, i even, we can define a pseudo spin-1/2 operator $\vec{\sigma}_i$ that acts on this dimer with the identification $|ST_0\rangle \equiv |\downarrow\rangle$ and $|T_0S\rangle \equiv |\uparrow\rangle$. An effective Hamiltonian can then be derived using standard many-body perturbation theory. The result depends on λ. If $\lambda > 0$, then the perturbation is lifted to first order in α, and the effective Hamiltonian reads

$$H_{eff}^{\lambda>0} = \alpha\lambda^2 \sum_{i \text{ even}} (\sigma_i^x \sigma_{i+2}^x + \frac{1}{4}) \qquad (9)$$

while if $\lambda = 0$ one has to go to second order perturbation theory to lift the degeneracy, and the effective Hamiltonian reads:

$$H_{eff}^{\lambda=0} = -\alpha^2 \sum_{i \text{ even}} (\sigma_i^x \sigma_{i+2}^x + \frac{1}{4}) \qquad (10)$$

Several remarks can be made about these results: First of all, the effective Hamiltonian is always an Ising model to the first non–vanishing order in perturbation theory. Second, the effective Ising model is antiferromagnetic if $\lambda > 0$ and ferromagnetic if $\lambda = 0$. These models are of course related by a simple transformation, but we expect to have a transition line between these cases in the (α, λ)–plane along which the effective Hamiltonian presumably takes a more complicated form. Finally, and more importantly, we obtain an Ising model in terms of $\sigma_i^x = (\sigma_i^+ + \sigma_i^-)/2$, *not* σ_i^z. So the eigenstates must be written in terms of the eigenstates of σ_i^x, namely $(|ST_0\rangle + |T_0S\rangle)/\sqrt{2}$ and $(|ST_0\rangle - |T_0S\rangle)/\sqrt{2}$. They are thus of the general form $2^{-L/4}\prod_{i\ \mathrm{even}}(|ST_0\rangle_i \pm |T_0S\rangle_i)$.

Let us now briefly discuss the low-energy properties. Quite generally, we expect to have a two-fold degenerate groundstate, and a gapped excitation spectrum. More specifically, the groundstates are given by

$$|GS\pm\rangle = 2^{-L/4}\prod_{i\ \mathrm{even}}(|ST_0\rangle_i \pm |T_0S\rangle_i) \qquad (11)$$

in the ferromagnetic case, and by

$$|GS\pm\rangle = 2^{-L/4}\prod_{i\ \mathrm{even}}(|ST_0\rangle_i \pm (-1)^{i/2}|T_0S\rangle_i) \qquad (12)$$

in the antiferromagnetic case. The first excitations are obtained by replacing $(|ST_0\rangle - |T_0S\rangle)/\sqrt{2}$ (resp. $(|ST_0\rangle + |T_0S\rangle)/\sqrt{2}$) by $(|ST_0\rangle + |T_0S\rangle)/\sqrt{2}$ (resp. $(|ST_0\rangle - |T_0S\rangle)/\sqrt{2}$) in one of these groundstates with energy $\alpha^2/2$ in the ferromagnetic case and $\alpha\lambda^2/2$ in the antiferromagnetic case. So there is indeed a gap in the spectrum. More importantly, it is clearly impossible to separate spin and orbital degrees of freedom since $(|ST_0\rangle + |T_0S\rangle)/\sqrt{2}$ and $(|ST_0\rangle - |T_0S\rangle)/\sqrt{2}$ are not eigenstates of $(\vec{S}_i + \vec{S}_{i+1})^2$ or of $(\vec{\tau}_i + \vec{\tau}_{i+1})^2$, and the excitations are neither spin excitations nor orbital excitations. They are transitions between resonating valence-bond states that intimately mix spin and orbital degrees of freedom.

It is also interesting to note that the correlation functions on a strong bond (i even) $\langle \vec{S}_i.\vec{S}_{i+1}\rangle$, $\langle \vec{\tau}_i.\vec{\tau}_{i+1}\rangle$ and $\langle (\vec{S}_i.\vec{S}_{i+1})(\vec{\tau}_i.\vec{\tau}_{i+1})\rangle$ are all negative, as in the SU(4) symmetric case, which excludes mean-field theory as a good starting point for the same reasons (see Ref. [6]).

Discussion: Coming back to the original problem of the nature of the excitations in the SU(4) symmetric model, let us put our results in perspective. In both cases studied above, exact results have been obtained, and the low–energy excitations are neither spin nor orbital excitations, but involve both spin and orbital degrees of freedom on an equal footing. This is a clear indication of the breakdown of mean-field theory. It strongly suggests that the model of Eq. (1) also possesses such low–lying excitations. In particular, the operators $\alpha_i^\pm = S_i^\pm \tau_i^\pm$ and $\beta_i^\pm = S_i^\pm \tau_i^\mp$ of the XY case are linear combinations of the operators $S^\alpha \tau^\beta$ which can be seen as generators of the SU(4) algebra (see Ref. [5]), and it is likely that at least part of the low-lying modes of the SU(4) symmetric model will be predominantly built on these generators and will retain the mixed character observed here. Besides, the fact that the correlation functions $\langle \vec{S}_i.\vec{S}_{i+1}\rangle$, $\langle \vec{\tau}_i.\vec{\tau}_{i+1}\rangle$ and $\langle (\vec{S}_i.\vec{S}_{i+1})(\vec{\tau}_i.\vec{\tau}_{i+1})\rangle$ are all negative on a given bond appears in the XXZ case as a direct consequence of the local degeneracy between the states (spin singlet × orbital triplet) and (spin triplet × orbital singlet). So the picture that emerges is that the symmetry between spin and orbital degrees of freedom has dramatic consequences on the low–lying excitations: The system is not able to choose between spin or orbital singlets or triplets, and the excitations are an intricate mixture of spin and orbital degrees of freedom.

To complete the picture, it will be useful to study the XXZ model in the whole parameter range $0 \le \alpha, \lambda \le 1$. The main issues are: i) The evolution of the spectrum along the line $(\alpha = 1, \lambda = 0) \to (\alpha = 1, \lambda = 1)$ joining the XY case and the model of Eq. (1); ii) The number of low–lying modes, and in particular the presence of a gap as a function of α and λ; iii) The nature of the effective model in the limit $\lambda = 1$, $\alpha \ll 1$. Work is in progress along these lines.

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